Optical Materials 76 (2018) 388-392

Contents lists available at ScienceDirect

**Optical Materials** 

journal homepage: www.elsevier.com/locate/optmat

# Tunable terahertz reflection spectrum based on band gaps of GaP materials excited by ultrasonic

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#### A R T I C L E I N F O

Article history: Received 15 November 2017 Received in revised form 4 January 2018 Accepted 5 January 2018

Keywords: Terahertz Ultrasonic GaP materials Polariton Reflection

#### ABSTRACT

Tunable terahertz (THz) reflection spectrum, ranged from 0.2 to 8 THz, in band gaps of gallium phosphide (GaP) materials excited by ultrasonic is investigated in the present paper, in which tunable ultrasonic and terahertz wave collinear transmission in the same direction is postulated. Numerical simulation results show that, under the acousto-optic interaction, band gaps of transverse optical phonon polariton dispersion curves are turned on, this leads to a dis-propagation of polariton in GaP bulk. On the other side, GaP material has less absorption to THz wave according to experimental studies, as indicates that THz wave could be reflected by the band gaps spontaneously. The band gaps width and acousto-optic coupling strength are proportional with ultrasonic frequency and its intensity in ultrasonic frequency range of 0-250 MHz, in which low-frequency branch of transverse optical phonon polariton dispersion curves demonstrate periodicity and folding as well as. With the increase of ultrasonic frequency, frequency of band gaps sconverge to the restrahlen band infinitely with frequency of ultrasonic exceeding over 250 MHz, total reflectivity of which is attenuated. As is show above, reflection of THz wave can be accommodated by regulating the frequency and its intensity of ultrasonic frequency. Relevant technology may be available in tunable THz frequency selection and filtering.

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# 1. Introduction

Terahertz radars [1,2] as the detection system of automotive still have not detailed report at present, one of the technology is THz selector technology. In recent years, the academic departments over the world have paid high attention to THz electromagnetic [3]. THz generation and detection technology has gained break through, meanwhile, the detection technology has been widely studied. In 2000,I. H. Libon achieved the THz selector by using superlattice structure quantum well [4]. In 2003, Stephan Biber studied the THz gating-selector using grating selector [5].

Superlattice or grating selector would be relatively easy to implement, whereas the frequency is limited to in the lowfrequency range (GHz) and the selector peripheral equipment is complex. Therefore, the resonance acousto-optic effect (RAOE) was

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simulated by P. St. J. Russell who substituted a Bragg reflector with periodic modulation superimposed for lattice polarization field [6]. P. V. Santos group modulated a photonic crystal selector using acoustic surface wave by citing RAOE in 2001 [7]. Photonic crystals [8] are immutable structure therefore could not be appropriate for tunable terahertz selector. And on this basis, A. L. Ivanov research group studied THz wave Bragg reflection of cuprous chloride (CuCl) crystal by analyzed RAOE theory [9].

In this paper, we studied the tunable terahertz reflection spectrum based on volume phase grating of GaP material. We calculated the parameters of GaP material by using the density functional theory (DFT) method [10]. The volume-phase grating in GaP material is formed by the tunable ultrasonic on the account of elastooptical effect. In the acousto-optic diffraction experiment, we demonstrated that the volume phase grating meet the Bragg condition and the acousto-optic constants change with the ultrasonic frequency and intensity. According to the results of ab-initio calculation methods, GaP crystal has hardly any absorption peaks in the 0.2–8 THz range. Band gaps appeared in transverse optical (TO) - phonon polariton (TOPP) dispersion curve driving by the



**Optical** Materia



volume-phase grating, and THz wave are forbidden for transmission at these band gaps position. Hence, THz wave would be reflecting with the incident light frequency equals the gaps based on collinear wave propagation method. In this paper, the modified TOPP dispersion equations and reflection equations are proposed. The reflectance spectra by numerical simulation demonstrated that THz reflection selector is feasible by adjusting the frequency of ultrasonic.

## 2. Research method

In this paper, the frequency spectrum of GaP materials sheet had been detected by using THz time-domain spectroscopy (THz-TDS). THz pulse was generated by gallium arsenide photoconductive switch. Femtosecond laser is mode-lock Ti-Sapphire lasers with pulses width is 50fs and wavelength is 820 nm (electrode gap: 50  $\mu$ m, bias voltage: 13 V, pump power: 50 mW) [11]. The phonon frequency (experimental value) is detected by using the laser Raman spectrometer.

The phonon frequency (calculated value) and other parameters of the cubic zinc-blende structure GaP crystal are calculated using the DFT method. The norm-conserving and the ultrasoft pseudo-potential method are respectively applied to the phonon frequency and optical/elastic parameters [12,13]. Super-cell with A:B:C = 2:2:1 is to improve the calculation speed and accuracy, respectively.

## 3. Result and discussion

## 3.1. Terahertz properties of GaP materials

According to the first principle method, the absorptivity ( $\alpha$ ) and the reflectivity (R) of GaP crystal are calculated. In 0.2–8 THz range, the absorption spectrum without absorption spike, the refractive index is 3.45 and the reflectance spectrum without reflection spike with the reflectivity is 0.295.

The terahertz frequency spectrum of GaP material is obtained by using the THz-TDS system which is shown in Fig. 1. Fig. 1(a) is the THz time-domain spectrum, main-peak of GaP crystal curve (violet square line) with weak attenuation delayed 6ps than reference curve (green solid line).

Fig. 1(b) is the frequency spectrum, the amplitude of GaP crystal smaller than the reference in 0.2–1.6 THz, and the spectrum dips (0.56 THz, 1.11 THz, 1.23 THz, 1.41 THz, 1.60 THz) are due to water vapor absorption of terahertz waves [14,15]. The inset figure is the refractive index of GaP, real part (pink solid line) and imaginary part (black thin line) of refractive index proved that GaP crystal has no obvious absorption spikes and have high transmittance in 0.2–1.6 THz range. Combined with the results of the first principle calculation (in the inset figure, real part: blue sphere scatter, imaginary part: orange square scatter), GaP crystal can be used as a THz selector.

#### 3.2. Phonon resonant frequency

The coefficient of the cubic phonon anharmonicity is so much bigger than the quartic of the cubic structure GaP crystal, the quartic phonon anharmonicity resonance would be to ignore in this study. There is one peak in the reflectance spectrum caused by acoustical-phonon transition within the volume-phase grating, therefore, the advantage of this design need not the secondary selector. According to the lattice vibration theory, the phonon frequency of the wave vector to meet positive value [16]. For the GaP crystal of semiconductor materials, the thermal conductivity mainly depends on the carrier concentration, and lattice vibration



**Fig. 1.** Measured terahertz pulses transmitted through the GaP crystal under the peak of the reference terahertz pulse, (a) THz time-domain spectrum. (b) frequency spectrum, the inset curves are real parts and imaginary parts of refractive index of GaP crystal.

plays an important role with the low carrier concentration. Fig. 2 is the phonon spectrum of GaP crystal calculated using the first-



**Fig. 2.** Phonon spectrum of GaP crystal calculated using the first-principles. The left curve is the phonon dispersion relation, the right curve is the total phonon density of states.

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